Sulfone, methyl pentafluorophenyl

651-85-4 | DTXSID30215403

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 104 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.14e-01

Confidence level: 5.04e-01

Nearest Neighbors from the Training Set

Image not found
Sulfone, methyl
pentafluorophenyl
Measured: 28.8
Predicted: 104

Image not found
Chlorothalonil
Measured: 1820
Predicted: 1300

Image not found
Chloranil
Measured: 209
Predicted: 259

Image not found
Fthalide
Measured: 2000
Predicted: 1600

Image not found
Dichlone
Measured: 9550
Predicted: 3350